

Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steven Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Schottky barrier formation at a carbon nanotube – metal junction

The hope of using carbon nanotubes as elements of electronic devices has advanced considerably toward becoming reality with recent demonstrations of CNT field-effect transistors (CNT-FETs). The issue of Schottky barrier formation at carbon nanotube contacts with metal leads is of crucial importance for nanotube-based electronic devices. Through first-principles total energy and electronic structure calculations within density functional theory, we have established that the junction between the metal covered part and the bare part of the CNT is responsible for the formation of a p-type Schottky barrier of ~ 0.4 eV, in excellent agreement with experiment. The figure shows metal-induced gap states, typical of Schottky barrier behavior for the (8,0) semi-conducting nanotube (orange atoms) in contact with a Pd metal ring (blue atoms).

